Lecturer . 2

Consider the following reaction:

$$2Na_3PO_4(aq) + 3Ba(NO_3)_2(aq) \rightarrow Ba_3(PO_4)_2(s) + 6NaNO_3(aq)$$

Suppose that a solution containing 3.50 grams of Na_3PO_4 is mixed with a solution containing 6.40 grams of $Ba(NO_3)_2$. How many grams of $Ba_3(PO_4)_2$ can be formed?

1. First we need to convert the grams of reactants into moles:

$$(3.50\,grams\,Na_3PO_4) * \left(\frac{1\,mole}{163.94\,grams}\right) = 0.0213\,moles\,Na_3PO_4$$

$$(6.40\,grams\,Ba(NO_3)_2) * \left(\frac{1\,mole}{261.34\,grams}\right) = 0.0245\,moles\,Ba(NO_3)_2$$

2. Now we need to define the stoichiometric ratios between the reactants and the product of interest ($Ba_3(PO_4)_2$):

$$2\ Na_3PO_4 \ \widehat{=}\ Ba_3(PO_4)_2$$

$$3\ Ba\ (NO_3)_2 \ \widehat{=}\ Ba_3(PO_4)_2$$

3. We can now determine the moles of product that would be formed if reactant were to be consumed in its entirety during the course of the reaction:

$$(0.0213\,moles\,Na_3PO_4) * \left(\frac{Ba_3(PO_4)_2}{2Na_3PO_4}\right) = 0.0107\,moles\,Ba_3(PO_4)_2$$

$$(0.0245\,moles\,Ba\,(NO_3)_2) * \left(\frac{Ba_3(PO_4)_2}{3Ba\,(NO_3)_2}\right) = 0.0082\,moles\,Ba_3(PO_4)_2$$

4. The limiting reactant is the Ba $(NO_3)_2$ and we could thus make at most 0.0082 moles of the $Ba_3(PO_4)_2$ product.

5. 0.0082 moles of the $Ba_3(PO_4)_2$ product would be equal to:

$$(0.0082\,moles\,Ba_3(PO_4)_2) * \left(\frac{601.93\,grams}{1\,mole\,Ba_3(PO_4)_2}\right) = 4.94\,grams$$

Theoretical yields

The quantity of product that is calculated to form when all of the limiting reactant is consumed in a reaction is called the theoretical yield.

The amount of product actually obtained is called the *actual yield*.

Actual yield < Theoretical yield

for the following reasons:

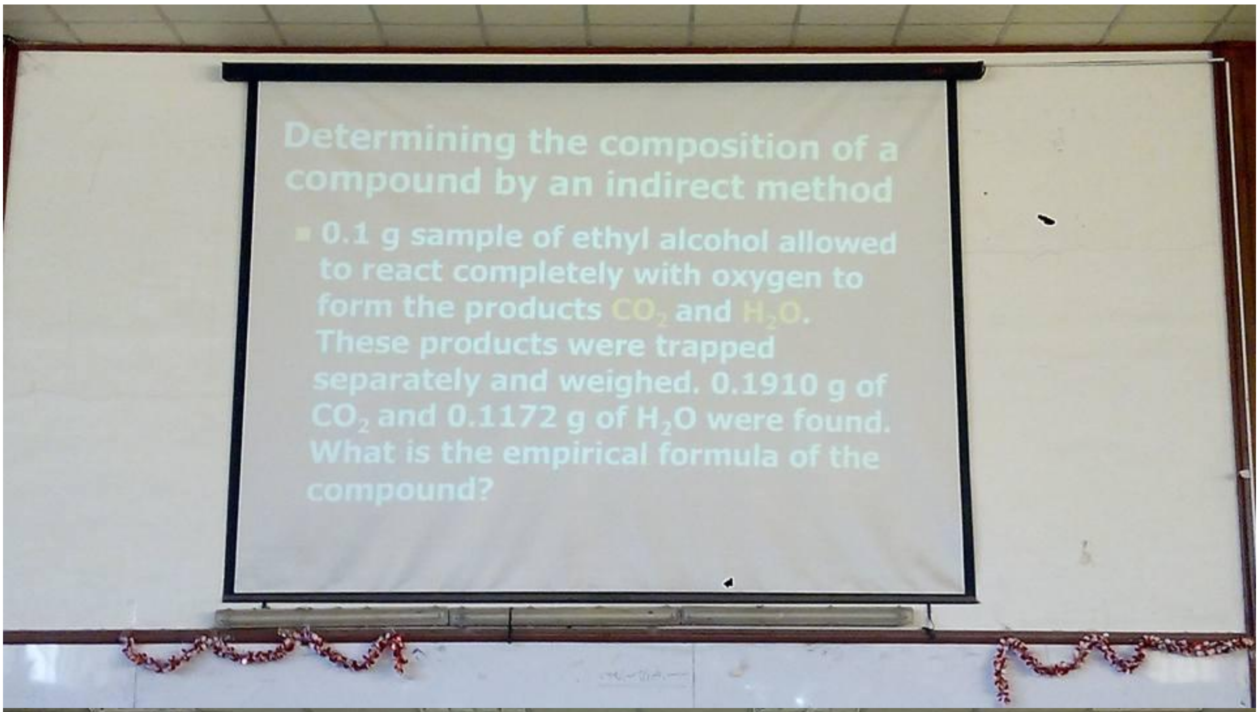
- **for some reason not all the reactants may react**
- **there may be some significant *side reactions***
- **physical recovery of 100% of the sample may be impossible (like getting all the peanut butter out of the jar)**

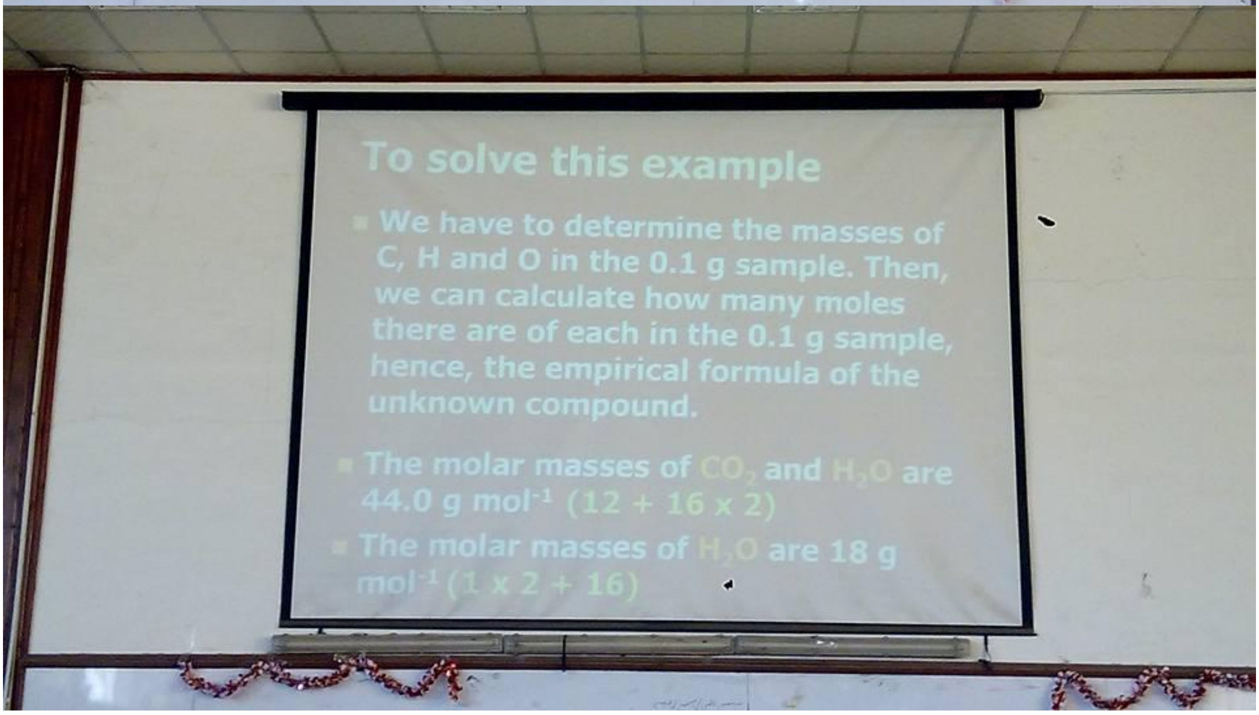
The *percent yield* of a reaction relates the actual yield to the theoretical yield:

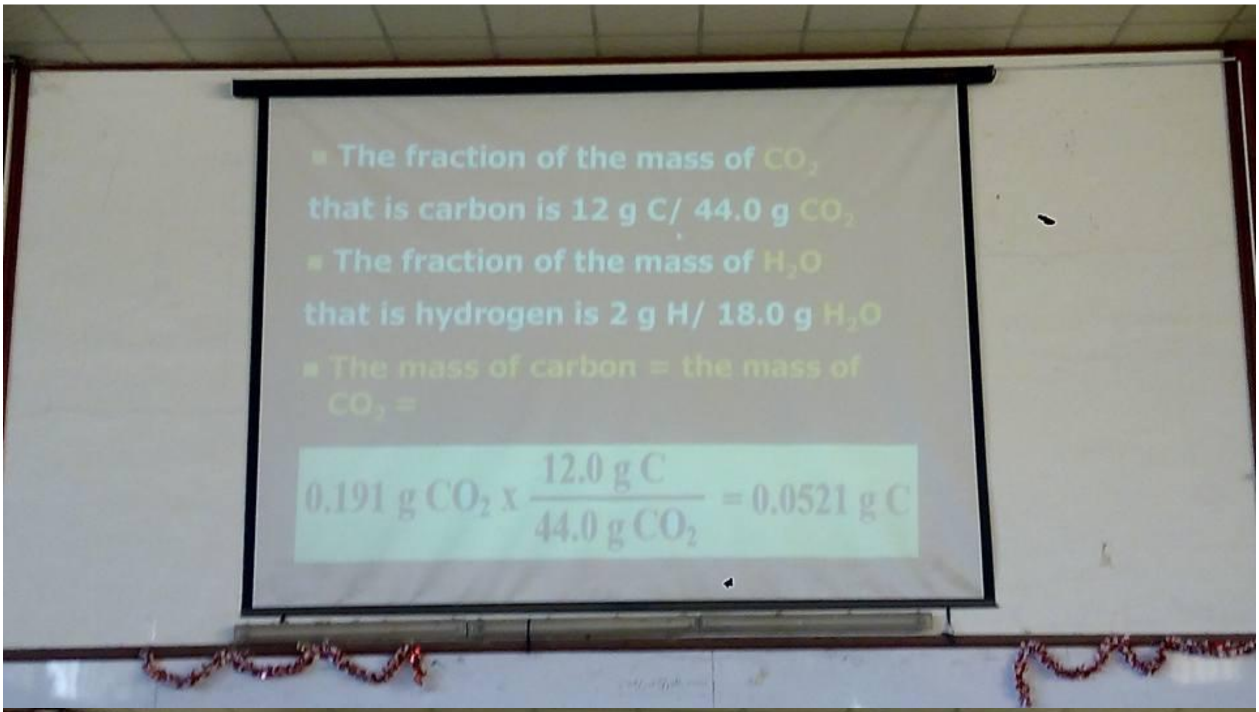
$$\text{Percent yield} = \left(\frac{actual\ yield}{theoretical\ yield}\right) \times 100$$

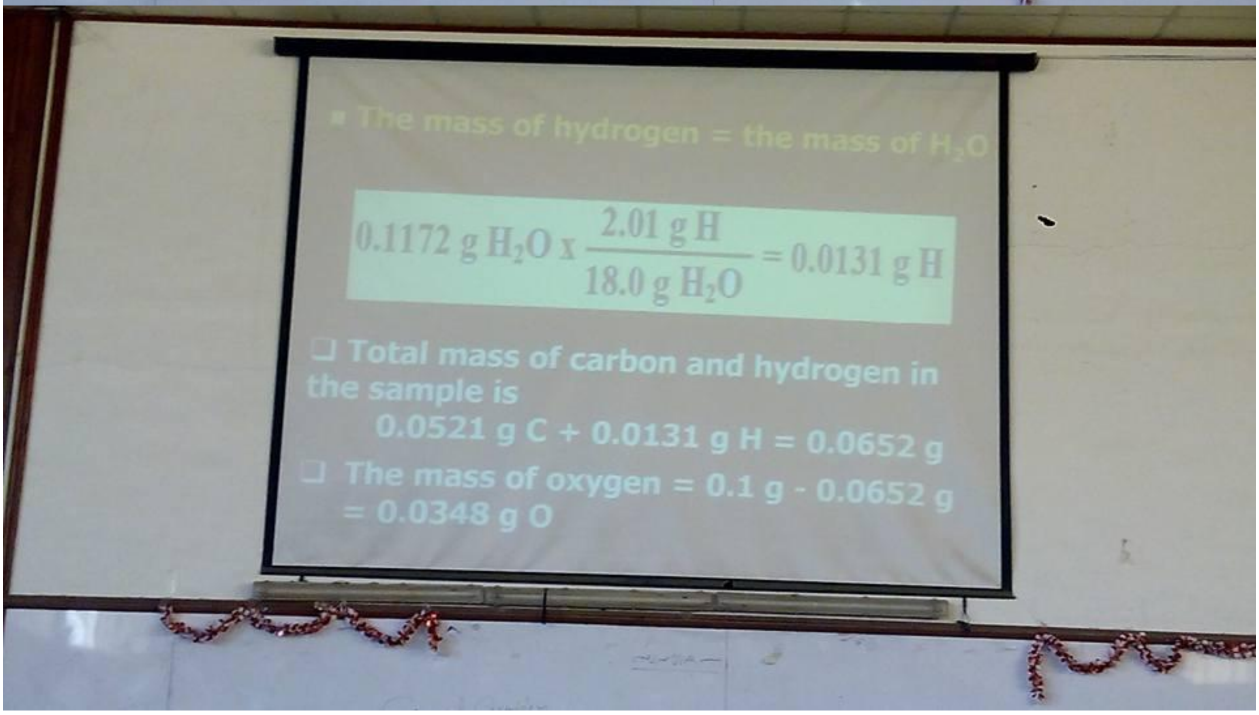
For example, in the previous exercise we calculated that 4.94 grams of $Ba_3(PO_4)_2$ product should be formed. This is the theoretical yield. If the actual yield were 4.02 grams the percent yield would be:

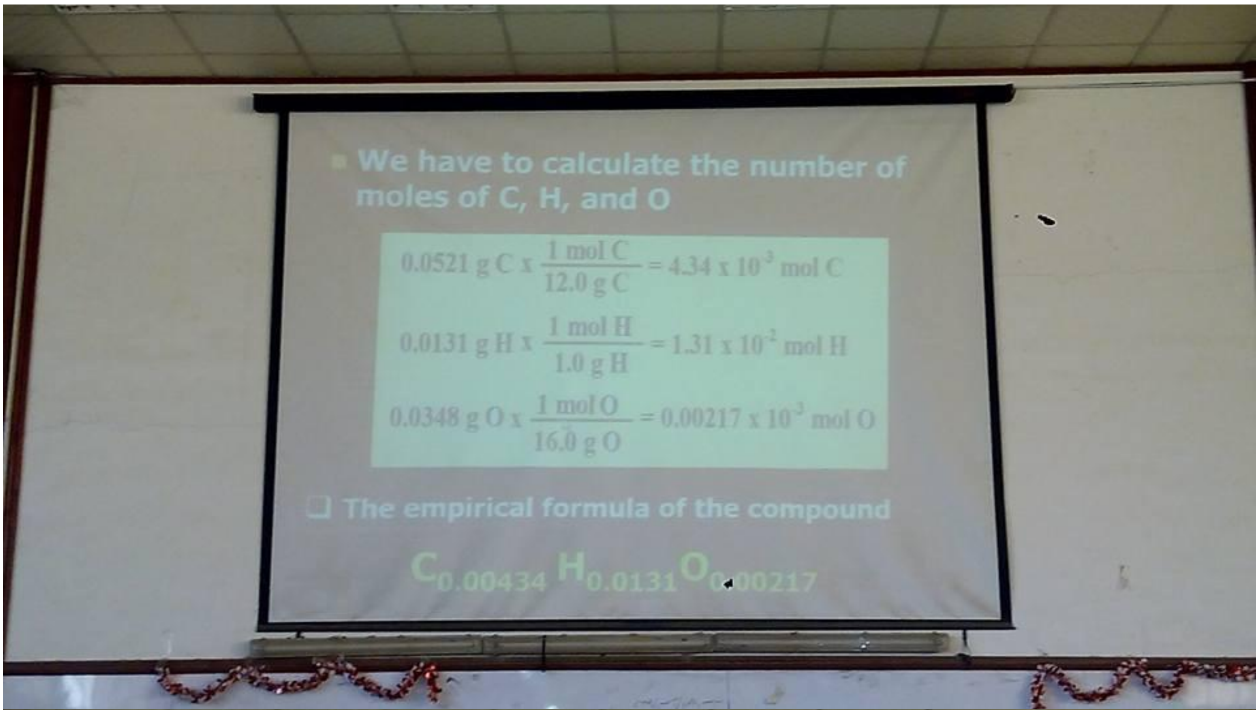
$$\text{Percent yield} = \left(\frac{4.02 grams}{4.94 grams}\right) \times 100 = 81\%$$

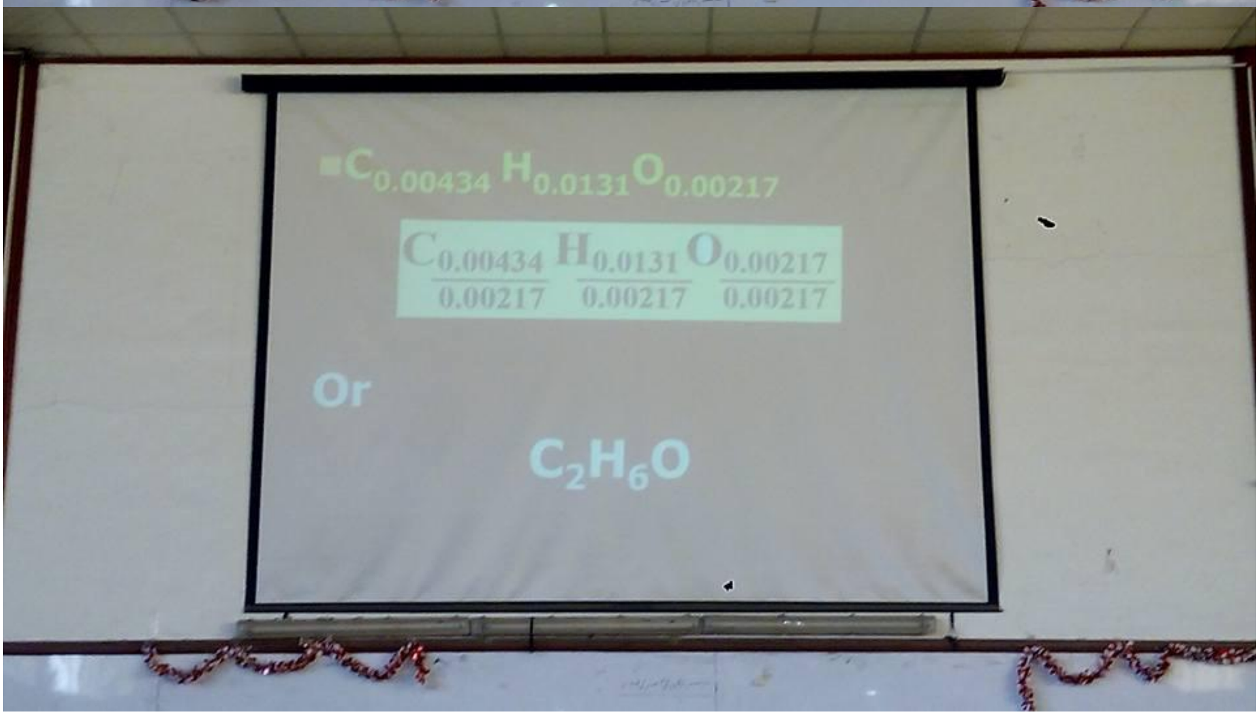

Determining the composition of a compound by an indirect method
0.1 g sample of ethyl alcohol allowed to react completely with oxygen to form the products CO2 and H2O. These products were trapped separately and weighed. 0.1910 g of CO2 and 0.1172 g of H2O were found. What is the empirical formula of the compound?


To solve this example
We have to determine the masses of C, H and O in the 0.1 g sample. Then, we can calculate how many moles there are of each in the 0.1 g sample, hence, the empirical formula of the unknown compound.
The molar masses of CO2 and H2O are 44.0 g mol-1 (12 + 16 x 2)
The molar masses of H2O are 18 g mol-1 (1 x 2 + 16)

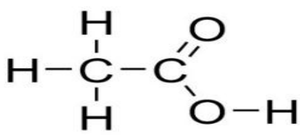

The fraction of the mass of CO_2
that is carbon is 12 g C/ 44.0 g CO_2
The fraction of the mass of H_2O
that is hydrogen is 2 g H/ 18.0 g H_2O
The mass of carbon = the mass of CO_2 =
$0.191\ g\ CO_2 \times \frac{12.0\ g\ C}{44.0\ g\ CO_2} = 0.0521\ g\ C$


The mass of hydrogen = the mass of H_2O
$0.1172\ g\ H_2O \times \frac{2.01\ g\ H}{18.0\ g\ H_2O} = 0.0131\ g\ H$
Total mass of carbon and hydrogen in the sample is
0.0521 g C + 0.0131 g H = 0.0652 g
The mass of oxygen = 0.1 g - 0.0652 g
= 0.0348 g O





<u>Chemical formula</u>

- **Empirical formula : NaCl , H_20 , CH_2**
- **Molecular formula : The actual number of each kind of atom found in a molecule such as H_20 , C_3H_6**
- **Structural formula :** 

Molecular Formula

Molecular weights as multiples of the empirical formula

formula	molecular formula
CH_2	$14 = 1 \times 14.0$
C_2H_4	$28 = 2 \times 14.0$
C_3H_6	$42 = 3 \times 14.0$
C_4H_8	$56 = 4 \times 14.0$
C_nH_{2n}	$N \times 14.0$

■ Example: A colorless liquid used in rocket engines, whose empirical formula is NO_2, has a molecular formula of 92.0, what is the molecular formula?

■ Solution page 33

Aqueous Reactions and Solution Stoichiometry

Solution Composition

Water possesses many unusual properties. One of the most important properties of water is its ability to dissolve a wide variety of substances.

Solutions in which water is the dissolving medium are called *aqueous solutions*.

Limestone caves, for example, are formed by the dissolving action of water, and dissolved CO_2, on solid Calcium Carbonate ($CaCO_3$).

The dissolved mineral is then deposited as stalagtites and stalagmites as the water evaporates: $CaCO_3(s) + H_2O(l) \rightarrow CO_2(aq) + Ca(HCO_3)_2(aq)$

stalactites and stalagmites

Many physiological chemical reactions occur in aqueous solutions.

How do we express solution composition?

What are the chemical forms in which substances occur in aqueous solutions?

Solution Composition

A *solution* is a homogenous mixture of two or more substances, consisting of :

1. **The *solvent* - usually the substance in greater concentration**
2. **The other component(s) is (are) called the solute(s) - they are said to be *dissolved* in the solvent**

When a small amount of NaCl is dissolved in a large quantity of water, we refer to the water as the *solvent* and the NaCl as the *solute*.

<u>Molarity</u>

The term *concentration* is used to indicate the amount of solute dissolved in a given quantity of solvent or solution.

The most widely used way of quantifying concentration in chemistry is *molarity*.

The *molarity* (symbol M) of a solution is defined as the number of moles of solute in a liter volume of solution:

$$Molarity = \frac{moles \quad solute}{volume \quad solution(liters)}$$

For example, *A1.0 molar solution (1.0 M) contains 1.00 mol of solute in every liter of solution*.

What is the molarity of a solution made by dissolving 20 grams of NaCl in 100 mls of water?

$$20 grams NaCl * \left(\frac{1 mol}{58.5 grams}\right) = 0.34 moles NaCl$$

$$\left(\frac{0.34 moles NaCl}{0.1 liter}\right) = 3.4 moles / liter = 3.4$$

M solution

If we know the molarity of a solution we can calculate the number of moles of solute in a given volume. Thus, molarity is a conversion factor between volume of solution and moles of solute:

Calculate the number of moles of $CaCl_2$ in 0.78 liters of a 3.5 M solution:

$$\left(\frac{3.5 moles CaCl_2}{1 liter}\right) * 0.78 liters = 2.73 moles$$

$CaCl_2$

How many liters of a 2.0 M solution of HNO_3 do we need to have 5 moles of HNO_3?

$$\left(\frac{1 liter}{2 moles}\right) * 5 moles = 2.5 liters$$

Note: we had to invert the stock solution (i.e. convert to liters per mole) to be able to calculate the needed volume (i.e. to keep the dimensional analysis correct)

Dilution

For convenience, solutions are either purchased or prepared in concentrated stock solutions which must be *diluted* prior to use.

When we take a sample of a stock solution we have a certain number of *moles* of molecules in that sample.

Dilution alters the molarity (i.e. *concentration*) of the solution but *not the total number of moles of molecules in the solution* (in other words, dilution does not create or destroy molecules).

One of the standard equations for determining the effects of dilution upon a sample is to set up an equation comparing *(concentration)*(volume)* before and after dilution.

Since *(concentration)*(volume)* gives us the *total number of moles in the sample*, and since this *does not change*, this value before and after dilution are equal:

(concentration)*(volume) = (concentration)*(volume)

(moles/liter)*(liter) = (moles/liter)*(liter)

moles = moles

■ **Example: How much of a 5 M stock solution of NaCl will you need to make up 250 mls of a 1.5 M solution?**

$$\left(\frac{5 moles}{liter}\right)*\left(X\ liters\right)=\left(\frac{1.5 moles}{liter}\right)*\left(0.25\ liters\right)$$

$$X\ liters=\left(\frac{1.5 moles}{liter}\right)*\left(0.25\ liters\right)*\left(\frac{liter}{5 moles}\right)$$

X liters = 0.075 liters (or 75 mls)

Thus, we would need 0.075 liters of our 5M NaCl stock solution. The rest of the 0.25 liter volume is made up by the addition of water:

0.25 liters - 0.075 liters = 0.175 liters

So we would take 0.075 liters of stock 5M NaCl solution and add to that 0.175 liters of water for a final volume of 0.25 liters with a final concentration of 1.5 moles/liter (i.e. 1.5 M)

What is the concentration of water?

Molecular weight of H_2O = 18.0g/mole

Density of H_2O = 1g/ml or 1000g/L

$$\left(\frac{1mole}{18.0g}\right)*\left(\frac{1000g}{L}\right) = 55.6M$$

Pure water is 55.6 M H_2O

Aqueous Reactions and Solution Stoichiometry

For balanced chemical equations involving solutions we calculate the number of moles by knowing the concentration (moles/liter, or Molarity) and volume (in liters).

■ Example: How many moles of water form when 25.0 mls of 0.100 M HNO_3 (nitric acid) solution is completely neutralized by NaOH (a base)?

1. Let's begin by writing the balanced equation for the reaction:

$$HNO_3(aq) + NaOH(aq) \rightarrow NaNO_3(aq) + H_2O(l)$$

2. The stoichiometric relationship between HNO_3 and H_2O is $HNO_3 \simeq H_2O$, therefore, for one mole of HNO_3 that is completely consumed (i.e. neutralized) in the reaction, one mole of H_2O is produced.

3. How many moles of HNO_3 are we starting with?

$$(.025liters)*\left(\frac{0.100moles}{liter}\right) = 0.0025moles$$ **HNO_3**

4. Therefore, we should have 0.0025 moles of H_2O produced

Titrations

How can we know the concentration of some solution of interest?

The answer is the method of *titration.*

In titration we will make use of a *second solution* known as a *standard solution* which has the following characteristics:

1. **The second solution contains a chemical which reacts in a defined way, with *known stoichiometry,* with the solute of the first solution**

2. **The *concentration* of the solute in this second solution is *known*.**

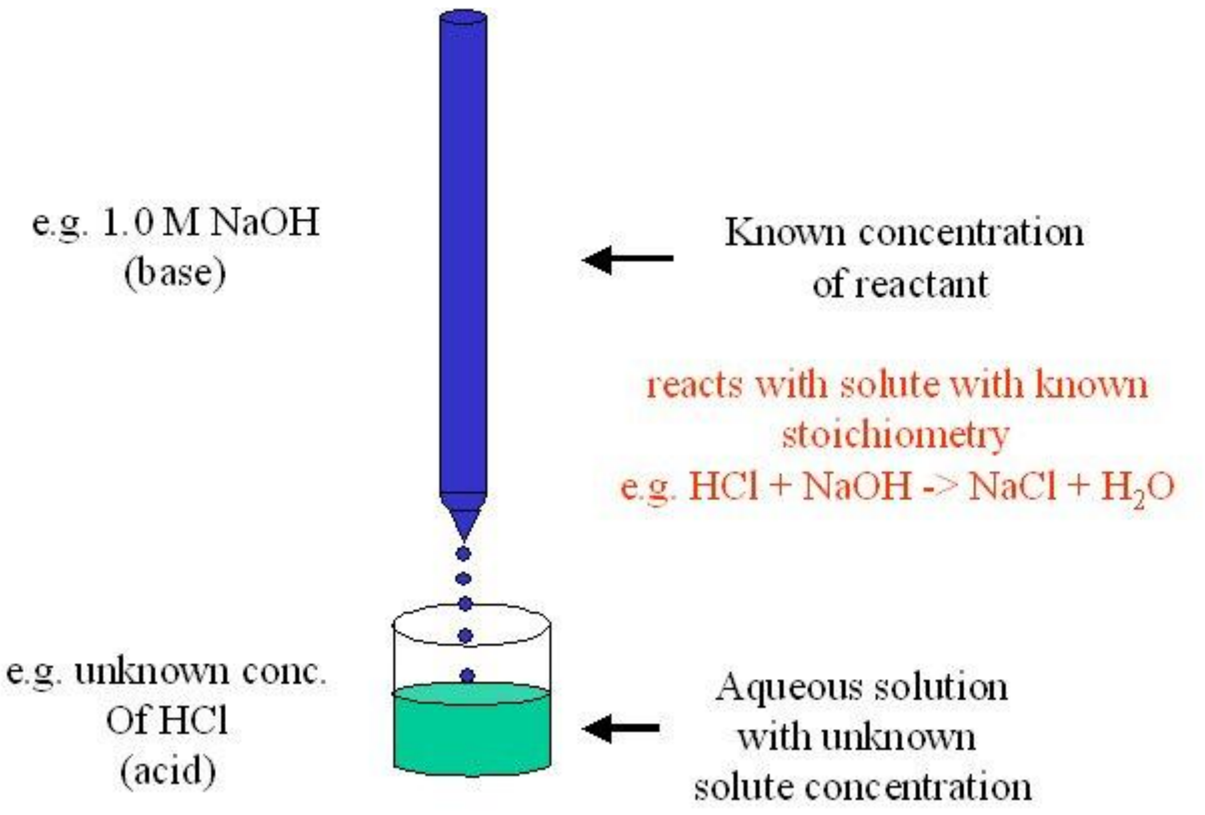
<u>Classic titrations include so-called acid-base titrations.</u>

In these experiments a solution of an acid with an unknown concentration is titrated with a solution of known concentration of base (or *vice versa*).

For example, we may have a solution of hydrochloric acid (HCl) of unknown concentration and a standard solution of NaOH. To a fixed amount of the HCl solution is added incremental amounts of the NaOH solution until the acid is completely neutralized - i.e. a stoichiometrically equivalent quantity of HCl and NaOH have been combined.

<u>Titration</u>

A stoichiometry equivalence quantity for example of HCL and NaOH have been combined.



This is known as the *equivalence point* in the titration.

By knowing the concentration of the standard solution, and the amount added to achieve stoichiometric equivalency, we can determine the amount of moles of HCl in the original sample volume.

How do we know when we have reached the equivalence point in such a titration experiment?

In this type of acid-base titration, so called *indicator-dyes* are used. For example *phenolphthalein* is colorless in acidic solutions and turns red in basic solutions. Thus, in the above experiment we will add a small amount of this indicator-dye and add base until we barely begin to see a color change to red.

■ Example: 25 mls of a solution of HCl with an unknown concentration is titrated with a standard solution of 0.5 M NaOH.

The phenolphthalein indicator dye begins to turn color after the addition of 2.8 mls of standard solution. What is the concentration of the HCl?

Balanced equation for the reaction:

$$HCl + NaOH \rightarrow NaCL + H_2O$$

$$(0.0028 liters)*\left(\frac{0.5 moles}{liter}\right) = 0.0014 moles$$ **of NaOH was added**

0.0014 moles of NaOH was added Since the stoichiometry of the NaOH and HCl is 1:1, the sample of HCl must have contained 0.0014 moles of HCl. The concentration of the HCl solution is therefore:

$$\left(\frac{0.0014 moles HCl}{0.025 liters}\right) = 0.056 moles/liter$$ **, or 0.056 M**
